Numerical Weather Prediction

Error covariance matrices having sinusoidal eigenvectors II: non-cyclic and mixed domains

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Abstract

The quest continues for conditions under which matrices representing homogeneous, symmetric error covariance have sinusoidal eigenvectors. Infinite, semi-infinite and finite non-cyclic domains are investigated, as well as domains that are cyclic in one or more directions but not in others. As in Part I, continuous cases are examined by simple-minded trial solution of integral equations. The results found in Part I for cyclic domains have analogues in infinite, non-cyclic domains: sinusoidal eigenfunctions are ubiquitous, and the associated eigenvalues are the Fourier cosine transforms of the covariance profile. For finite domains, the discrete problem involves matrices of Toeplitz rather than circulant type, and the occurrence of sinusoidal eigenvectors is far less common - as is readily understandable via a smoothing analogy. Nevertheless, some families of covariance profiles are identified that give sinusoidal eigenvectors (in the discrete problem, and sinusoidal eigenfunctions in the continuous problem). No examples are found of strictly sinusoidal eigenfunctions in semi-infinite domains. Cases giving sinusoidal eigenfunctions exist in mixed cyclic, non-cyclic domains such as the spherical annulus. Implications for the understanding of variational data assimilation schemes are discussed.

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1 Introduction

In Part I of this study (White and Healy 2004) it was noted that eigen-problems of error covariance matrices can be viewed as discretizations of certain integral eigen-problems, and that the eigenvectors (or eigenfunctions) are simple sinusoids if the covariance is homogeneous and symmetric and the domain periodic and Cartesian. Further, the eigenvalues are proportional to the Fourier cosine transform of the covariance profile. On a spherical surface, the corresponding eigen-problem yields spherical harmonic eigenfunctions, with eigenvalues proportional to the Legendre transform of the covariance profile. These results throw light on various data assimilation issues and procedures. The cases treated in Part I involved cyclic domains - whether infinite and Cartesian or compact and surface-spherical. Here in Part II we extend the search for sinusoidal eigenvectors to non-cyclic and mixed domains. Infinite non-cyclic domains are considered in section 2, finite domains in section 3, semi-infinite domains in section 4, and mixed cyclic, non-cyclic domains (such as that of the Earth's atmosphere) in section 5. Implications for the use and interpretation of data assimilation schemes are discussed in section 6, together with some suggestions for further work.

2 Infinite domains

As noted in Part I, the matrix eigenvalue problem

$$\mathbf{K}\mathbf{f} = \lambda\mathbf{f}, \tag{2.1}$$

in which $\mathbf{K}$ is an $N \times N$ matrix, $\mathbf{f}$ is an N-component eigenvector and λ is an eigenvalue, may be regarded as a uniform discretization of an integral eigenvalue problem of the form

$$\int_a^b K\,(X,\,x)\,f(x)\,dx = \lambda f(X). \tag{2.2}$$

Evaluation of the kernel function K in (2.2) at pairs of points leads to the elements of the matrix $\mathbf{K}$ in (2.1). The integration over x (for each X) in (2.2) is analogous to the action of each row of $\mathbf{K}$ on the column vector $\mathbf{f}$ in (2.1). This correspondence has been well known for a long time; see, for example, Courant and Hilbert (1962) and Mathews and Walker (1965).

Of particular relevance to homogeneous, symmetric covariance eigen-problems are cases in which the kernel $K(X,\,x)$ depends only on the difference between x and X:

$$\int_a^b K\,(|x - X|)\,f(x)\,dx = \lambda f(X). \tag{2.3}$$

($K\,(x - X)$ is called a displacement kernel. $K\,(|x - X|)$ is a symmetric displacement kernel.)

Having considered in Part I various examples of cyclic domains, we examine here the case of an infinite domain, so that (2.3) becomes

$$\int_{-\infty}^{\infty} K\,(|x - X|)\,f(x)\,dx = \lambda f(X). \tag{2.4}$$

Consider the left-hand side of (2.4) as the definition of a new function g:

$$g(X) = \int_{-\infty}^{\infty} K\,(|x - X|)\,f(x)\,dx. \tag{2.5}$$

To find eigenfunctions of (2.4), a trial approach may be applied to (2.5): (i) choose a promising form for the function f; (ii) evaluate the integral; (iii) look for conditions under which $g(X)$ has the same form as $f(X)$ - and hence the chosen form is an eigenfunction of (2.4).

With $f(x) = \cos kx$ and the substitution $z = x - X$, (2.5) becomes

$$g(X) = \int_{-\infty}^{\infty} K\,(|z|)\cos k(z + X)dz. \tag{2.6}$$

By expanding the cosine term as $\cos kz \cos kX - \sin kz \sin kX$ and noting the symmetry of $K\,(|z|)$ about $z = 0$, (2.6) may be re-written as

$$g(X) = \cos kX \int_{-\infty}^{\infty} K\,(|z|)\cos kzdz = 2\cos kX \int_0^{\infty} K\,(|z|)\cos kzdz. \tag{2.7}$$

Hence $f(x) = \cos kx$ is an eigenfunction of (2.5), and the associated eigenvalue is - apart from a constant factor - the Fourier cosine transform of the kernel function K.

With $f(x) = \sin kx$, the same experimental procedure leads from (2.5) to

$$g(X) = \sin kX \int_{-\infty}^{\infty} K(|z|) \cos kz dz = 2 \sin kX \int_{0}^{\infty} K(|z|) \cos kz dz. \tag{2.8}$$

So $f(x) = \sin kx$ is also an eigenfunction of (2.5), and it has the same eigenvalue as the eigenfunction $f(x) = \cos kx$.

The action of multiplying $f(x)$ by $K(|x - X|)$ and integrating over x in (2.4) and (2.5) may be regarded as a smoothing operation centred on X, with K playing the role of a weighting function. The eigenvalue problem (2.4) seeks those functions that survive the smoothing as regards form, and suffer only a change of amplitude. From this perspective - as noted in Part I for a cyclic domain - it is not surprising that the eigenfunctions of (2.4) in an infinite domain are sinusoids. A common problem in elementary signal processing is to find the effect of a symmetric smoother on a sinusoidal input; the result is also a sinusoid, but with altered (usually reduced) amplitude. In other words, sinusoids are eigenfunctions of the symmetric smoothing operator, and the eigenvalues represent the amplitude modifications.

The simplicity of these results is reminiscent of those obtained in Part I for a 1D cyclic domain; it seems that the 1D domain $-\infty < x < +\infty$ is a similar environment to the cyclic 1D domain for many purposes of covariance analysis. Arguably, the analysis in the infinite domain case is even more straightforward than in the cyclic case.

Extension to 2D and 3D infinite domains is straightforward if the covariance kernel is separable into symmetric factors. The eigenfunctions then are products of sinusoids, and the eigenvalues are transforms of the 2D or 3D kernel. If the kernel is radially symmetric, the relevant transform in 2D is the zero order Hankel transform, while in 3D it is a radially weighted Fourier transform.

3 Finite domains

We limit attention to 1D finite domains (though 2D and 3D cases are clearly of oceanographic relevance). On the basis of the smoothing analogy previously noted, we expect sinusoidal eigenvectors to occur much less commonly than in cyclic or infinite domains, since boundary effects will complicate the smoothing in their vicinity. Nevertheless, for some families of covariance profiles sinusoidal eigenvectors *are* found. A specific discrete case will be examined first (for more general results, see Appendix) and then some continuous cases.

(a) A 7×7 matrix of homogeneous, symmetric error covariance

Simpler cases than 7×7 turn out not to be typical of the general $N \times N$ problem, at least for odd N. The covariance matrix is the symmetric Toeplitz form

$$\mathrm{T}_7 = \begin{pmatrix} 1 & a & b & c & d & e & f \\ a & 1 & a & b & c & d & e \\ b & a & 1 & a & b & c & d \\ c & b & a & 1 & a & b & c \\ d & c & b & a & 1 & a & b \\ e & d & c & b & a & 1 & a \\ f & e & d & c & b & a & 1 \end{pmatrix} \tag{3.1}$$

in which the elements in any given diagonal are identical (see Golub and Van Loan (1996), p193). a, b, c, d, e and f represent the error covariance between points respectively Δx, $2\Delta x$, $3\Delta x$, $4\Delta x$, $5\Delta x$ and $6\Delta x$ apart in a 1D domain of length $6\Delta x$; see Figure 1. In the cyclic case we would have $d = c$, $e = b$ and $f = a$ (see Part I). We shall assume here only that $1 > a \geq b \geq c \geq d \geq e \geq f > 0$.

First, seek symmetric sinusoidal eigenvectors $\mathbf{x}_{sym}$ of the form

$$\mathbf{x}_{sym} = (\cos 3\alpha, \cos 2\alpha, \cos \alpha, 1, \cos \alpha, \cos 2\alpha, \cos 3\alpha)^T, \tag{3.2}$$

where α is as yet undetermined (and the superscript T indicates transposition). Our approach is simply to form $\mathbf{T}_7\mathbf{x}_{sym}$ and to find the conditions under which it is a constant multiple of $\mathbf{x}_{sym}$, i.e. $\mathbf{T}_7\mathbf{x}_{sym} = \lambda\mathbf{x}_{sym}$ where λ is the associated eigenvalue. From the fourth (central) components of $\mathbf{T}_7\mathbf{x}_{sym}$ and $\lambda\mathbf{x}_{sym}$ it follows that

$$\lambda = 1 + 2a\cos\alpha + 2b\cos 2\alpha + 2c\cos 3\alpha. \tag{3.3}$$

By considering the third (or the fifth) components of $\mathbf{T}_7\mathbf{x}_{sym}$ and $\lambda\mathbf{x}_{sym}$, with λ given by (3.3), we derive the requirement

$$d\cos 3\alpha = c\cos 4\alpha. \tag{3.4}$$

Given c and d, (3.4) may be regarded as a transcendental equation for α; sketching $\cos 3\alpha$ and $\cos 4\alpha$ makes clear that (3.4) has 4 solutions ($c \geq d$). From the second (or the sixth) components of $\mathbf{T}_7\mathbf{x}_{sym}$ and $\lambda\mathbf{x}_{sym}$ (with (3.3)) a further requirement is obtained:

$$d\cos 2\alpha + e\cos 3\alpha = b\cos 4\alpha + c\cos 5\alpha. \tag{3.5}$$

By multiplying (3.4) by $2\cos\alpha$, and using standard identities, it follows that (3.4) implies (3.5) if

$$c(c + e) = d(d + b). \tag{3.6}$$

Finally, from the first (or the seventh) components of $\mathbf{T}_7\mathbf{x}_{sym}$ and $\lambda\mathbf{x}_{sym}$ (with (3.3)):

$$d\cos\alpha + e\cos 2\alpha + f\cos 3\alpha = a\cos 4\alpha + b\cos 5\alpha + c\cos 6\alpha. \tag{3.7}$$

Manipulation shows that (3.7) is implied by (3.5) if

$$c(b + f) = d(a + e). \tag{3.8}$$

If conditions (3.6) and (3.8) are obeyed, then $\mathbf{T}_7$ has symmetric sinusoidal eigenvectors of the form (3.2), with eigenvalues given by (3.3) and α determined by (3.4).

The constants a, b, c, d, e, f do not generally obey (3.6) and (3.8), but cases exist in which they do. Such cases include:
(i) $b = a^2$, $c = a^3$, $d = a^4$, $e = a^5$, $f = a^6$ (*exponential*);
(ii) $a = 1 - \delta$, $b = 1 - 2\delta$, $c = 1 - 3\delta$, $d = 1 - 4\delta$, $e = 1 - 5\delta$, $f = 1 - 6\delta$ (*linear*);
(iii) $b = c = d = e = f = a$ (*uniform*).
Cases in which (3.6) and (3.8) are *not* obeyed include:
(iv) $b = a^2$, $c = a^9$, $d = a^{16}$, $e = a^{25}$, $f = a^{36}$ (*Gaussian*);

(v) $a = 1-\delta^2$, $b = 1-4\delta^2$, $c = 1-9\delta^2$, $d = 1-16\delta^2$, $e = 1-25\delta^2$, $f = 1-36\delta^2$ (*parabolic*);
(vi) $a = \delta\,(2-\delta)$, $b = \delta^2\,(2-\delta^2)$, $c = \delta^3\,(2-\delta^3)$, $d = \delta^4\,(2-\delta^4)$, $e = \delta^5\,(2-\delta^5)$, $f = \delta^6\,(2-\delta^6)$ (*double exponential*).
In cases (ii), (v) and (vi), δ is assumed positive but sufficently small that f remains positive. Continuous analogues of cases (i), (ii), (v) and (vi) will be studied in section 3(b).

Next, seek antisymmetric sinusoidal eigenvectors $\mathbf{x}_{asym}$ of $\mathbf{T}_7$ of the form

$$\mathbf{x}_{asym} = (\sin 3\alpha, \sin 2\alpha, \sin\alpha, 0, -\sin\alpha, -\sin 2\alpha, -\sin 3\alpha)^T. \tag{3.9}$$

The fourth components of $\mathbf{T}_7\mathbf{x}_{asym}$ and $\mathbf{x}_{asym}$ are both identically zero. The third (and the fifth) components of $\mathbf{T}_7\mathbf{x}_{asym}$ and $\lambda\mathbf{x}_{asym}$ are equal so long as the eigenvalue λ obeys

$$\lambda = 1 - b + 2(a-c)\cos\alpha + (b-d)(2\cos 2\alpha + 1). \tag{3.10}$$

Given (3.10), the second (and the sixth) components of $\mathbf{T}_7\mathbf{x}_{asym}$ and $\lambda\mathbf{x}_{asym}$ are equal if

$$(c-e)\sin 3\alpha = (b-d)\sin 4\alpha. \tag{3.11}$$

Given a, b, c and d, condition (3.11) may be regarded as a transcendental equation for α; it has 3 solutions. The first (and the seventh) components of $\mathbf{T}_7\mathbf{x}_{asym}$ and $\lambda\mathbf{x}_{asym}$ are equal if

$$(c-e)\sin 2\alpha + (d-f)\sin 3\alpha = (a-c)\sin 4\alpha + (b-d)\sin 5\alpha. \tag{3.12}$$

Condition (3.11) implies (3.12) if

$$(b-f)(b-d) = (c-e)(a-e). \tag{3.13}$$

(3.13) is the condition for antisymmetric sinusoidal eigenvectors to exist in the 7×7 problem. It is satisfied in the exponential, linear and uniform cases (i) - (iii) noted above, but not in the Gaussian case (iv) or the double exponential case (vi). Condition (3.13) *is* satisfied in the parabolic case (v) - thus showing that antisymmetric sinusoidal eigenvectors may exist when symmetric sinusoidal eigenvectors do not. (In deriving (3.13), $c \neq e$ was assumed. In case (iii), $c = e$, but (3.12) is satisfied identically, so (3.13) is not needed.)

Results for $N \times N$ generalizations of cases (i) - (iii) are given in the Appendix: sinusoidal eigenvectors occur in each.

(b) Continuous cases

It is convenient to move the origin so that the interval $x\,\epsilon\,[a,b]$ becomes $x\,\epsilon\,[-L,+L]$ (with $L = (b-a)/2$). The integral equation (2.3) then becomes

$$\int_{-L}^{L} K\left(|x-X|\right) f(x)\,dx = \lambda f(X). \tag{3.14}$$

Once again, an experimental approach is useful: (i) consider the new function g defined by

$$g(X) \equiv \int_{-L}^{L} K\left(|x-X|\right) f(x)\,dx; \tag{3.15}$$

(ii) assume a sinusoidal form for f; and (iii) find under what conditions (if any) $g(X)$ is of the same form as $f(X)$. With $z = x - X$, (3.15) becomes

$$g(X) = \int_{-(L+X)}^{L-X} K(|z|) f(z+X)\, dz. \tag{3.16}$$

We give results only for specific choices of symmetric kernel, but will offer some general speculations. We distinguish two types of symmetric kernel: *smooth* and *salient*. As illustrated in Figure 2, a smooth symmetric kernel $K(z)$ has a continuous gradient everywhere, and hence zero gradient at $z = 0$; while a salient symmetric kernel has a change of gradient at $z = 0$ (which is therefore a salient point of $K(z)$ - see Daintith and Nelson (1989)).

Piece-wise exponential kernel (salient)

With the kernel $K(|z|) = e^{-\alpha|z|}$, $\alpha > 0$, (sometimes called the Picard kernel) (3.16) becomes

$$g(X) = \int_{-(L+X)}^{0} e^{\alpha z} f(z+X)\, dz + \int_{0}^{L-X} e^{-\alpha z} f(z+X)\, dz. \tag{3.17}$$

The two integrals in (3.17) are contributions from the regions to the left and to the right of the salient point $z = 0$ in $K(|z|)$. See Figure 2.

With $f(x) = \sin kx$ in (3.17), use of

$$\left(\alpha^2 + k^2\right) \int e^{\alpha z} \sin k(z+X) dz = e^{\alpha z} \left[\alpha \sin k(z+X) - k \cos k(z+X)\right] \tag{3.18}$$

gives

$$\left(\alpha^2 + k^2\right) g(X) = 2\alpha \sin kX - 2\alpha e^{-\alpha L} \sinh \alpha X \left[\sin kL + \frac{k}{\alpha} \cos kL\right]. \tag{3.19}$$

$f(x) = \sin kx$ is thus an eigenfunction, with associated eigenvalue $2\alpha\left(\alpha^2 + k^2\right)^{-1}$, if the coefficient of $\sinh \alpha X$ in (3.19) vanishes. This occurs if kL obeys the transcendental equation

$$\sin kL + \frac{kL}{\alpha L} \cos kL = 0. \tag{3.20}$$

Equation (3.20) is of the form

$$\tan y + Cy = 0, \tag{3.21}$$

which has a countable infinity of solutions for $y\,(= kL)$, nine of which are tabulated, for 20 positive values of $C\,(= (\alpha L)^{-1})$, in Abramowitz and Stegun (1968) - see their p224.

With $f(x) = \cos kx$ and use of

$$\left(\alpha^2 + k^2\right) \int e^{\alpha z} \cos k(z+X) dz = e^{\alpha z} \left[\alpha \cos k(z+X) + k \sin k(z+X)\right], \tag{3.22}$$

the same procedure gives

$$\left(\alpha^2 + k^2\right) g(X) = 2\alpha \cos kX + 2k e^{-\alpha L} \cosh \alpha X \left[\sin kL - \frac{\alpha}{k} \cos kL\right]. \tag{3.23}$$

So $f(x) = \cos kx$ is an eigenfunction, with eigenvalue $2\alpha\left(\alpha^2 + k^2\right)^{-1}$, if kL obeys

$$\alpha L \cos kL = kL \sin kL. \tag{3.24}$$

This is of the form

$$\cot y = Cy, \tag{3.25}$$

which is a transcendental equation having a countable infinity of solutions, a number of which can also be found in Abramowitz and Stegun (1968) (see p 225).

Use of (3.22) shows that the eigenvalue $2\alpha\left(\alpha^2 + k^2\right)^{-1}$ is proportional to the standard Fourier cosine transform of the kernel $K\left(|z|\right) = e^{-\alpha|z|}$. Although the functional form of the eigenvalue is the same for both the symmetric and anti-symmetric eigenfunctions, the permitted values of k are not numerically identical (because they are determined by (3.24) in the former case and by (3.21) in the latter) and so the eigenfunctions are not degenerate.

Piece-wise linear kernel (salient)

For the kernel $K\left(|z|\right) = 1 - \alpha\,|z|$, with $2\alpha L \leq 1$ (stipulated so that K does not become negative within the domain), (3.16) becomes

$$g(X) = \int_{-L}^{L} f(x)\,dx + \alpha \int_{-(L+X)}^{0} z f(z+X)\,dz - \alpha \int_{0}^{L-X} z f(z+X)\,dz. \tag{3.26}$$

The first integral in (3.26) represents in its simplest form the contribution of the constant term in $K\left(|z|\right) = 1 - \alpha\,|z|$. The second and third integrals represent contributions from the regions to the left and to the right of the salient point $z = 0$ in K; see Figure 2. An important feature of (3.26) is that the integral $\int z f(z+X) dz$ (whatever it is) contributes twice with the same sign in the evaluations at $z = 0$; this reflects the salient character of K.

For $f(x) = \sin kx$ in (3.26), use of

$$k^2 \int z \sin k(z+X) dz = -kz \cos k(z+X) + \sin k(z+X), \tag{3.27}$$

gives

$$k^2 g(X) = 2\alpha \sin kX - 2\alpha kX \cos kL\ . \tag{3.28}$$

Thus $f(x) = \sin kx$ is an eigenfunction if

$$kL = \frac{\pi}{2}(2n+1), \quad n = 0, 1, 2, ... \tag{3.29}$$

These antisymmetric eigenfunctions form a countably infinite set whose values of k are spaced at intervals of exactly $\Delta k = \pi/L$ (independent of the quantity αL). The associated eigenvalues of (3.14) are $2\alpha/k^2$.

For $f(x) = \cos kx$ in (3.26), use of

$$k^2 \int z \cos k(z+X) dz = kz \sin k(z+X) + \cos k(z+X), \tag{3.30}$$

gives

$$k^2 g(X) = 2\alpha \cos kX + \frac{2}{L}\left[(1 - \alpha L)\, kL \sin kL - \alpha L \cos kL\right]\ . \tag{3.31}$$

Thus $f(x) = \cos kx$ is an eigenfunction, with eigenvalue $2\alpha/k^2$, if the term in the square backets in (3.31) vanishes, i.e. if kL obeys the transcendental equation

$$\cot kL = \left(\frac{1-\alpha L}{\alpha L}\right) kL\,. \tag{3.32}$$

Eq.(3.32) is of the form (3.25), with $C+1 = (\alpha L)^{-1}$; it has an infinity of solutions spaced at intervals of about $\Delta k = \pi/L$ in k.

Once again, although the functional form of the eigenvalues is the same for both the symmetric and anti-symmetric eigenfunctions, the allowed values of k are different and so the eigenfunctions are not degenerate.

Parabolic kernel (smooth)

With the kernel $K(|z|) = 1-\beta^2 z^2$ (we assume $2\beta L \leq 1$ so that K does not become negative within the domain), (3.16) becomes

$$g(X) = \int_{-L}^{L} f(x)\,dx - \beta^2 \int_{-(L+X)}^{L-X} z^2 f(z+X)\,dz. \tag{3.33}$$

The range of the second integral has not been split: $K(|z|) = 1-\beta^2 z^2$ is a smooth function.

Consider first the case $f(x) = \sin kx$. Upon use of

$$k^3 \int z^2 \sin k(z+X)dz = -k^2 z^2 \cos k(z+X) + 2kz \sin k(z+X) + 2\cos k(z+X), \tag{3.34}$$

(3.33) reduces after some manipulation to

$$k^2 g(X) = -4\beta^2 X\left[kL\cos kL - \sin kL\right]. \tag{3.35}$$

If kL obeys the transcendental equation

$$\tan kL = kL, \tag{3.36}$$

then $f(x) = \sin kx$ is an eigenfunction, and the corresponding eigenvalue is zero. Eq.(3.36) is of the form (3.21); it has a countable infinity of solutions, spaced at intervals of about $\Delta k = \pi/L$ in k. Thus the functions $f(x) = \sin kx$, with k satisfying (3.36), are a multiply degenerate set of eigenfunctions with zero eigenvalue.

A similar treatment for $f(x) = \cos kx$, using

$$k^3 \int z^2 \cos k(z+X)dz = k^2 z^2 \sin k(z+X) + 2kz\cos k(z+X) - 2\sin k(z+X), \tag{3.37}$$

leads to

$$k^3 g(X) = 2\sin kL\left[k^2 - \beta^2 k^2 (L^2+X^2) + 2\beta^2\right] - 4\beta^2 kL\cos kL. \tag{3.38}$$

Clearly, $f(x) = \cos kx$ is not an eigenfunction (assuming $k \neq 0$).

The existence of antisymmetric but not symmetric sinusoidal eigenfunctions in this case is consistent with the results of the 7×7 *parabolic* case (v) of section 3(b). Also, the existence of both antisymmetric and symmetric sinusoidal eigenfunctions with piece-wise exponential and piece-wise linear kernels is consistent with the results of the 7×7 *exponential* and *linear* cases (i) and (ii) of section 3(b). Analytical treatment of (3.16) with a Gaussian kernel is not straightforward, so we shall not investigate whether the indications of the 7×7 *Gaussian* case (iv) are borne out in the continuous problem. Instead we examine a tractable continuous problem for which the 7×7 discretization is the *double exponential* case (vi) of section 3(a).

A double exponential kernel (smooth)

Consider the kernel

$$K\left(|z|\right) = 2e^{-\gamma|z|} - e^{-2\gamma|z|} = 1 - \left(1 - e^{-\gamma|z|}\right)^2. \tag{3.39}$$

This "double exponential" kernel is non-negative, and its gradient smooth, for all z. To examine whether it allows sinusoidal eigenfunctions, we may evaluate $g(X)$ from (3.16) using results already obtained.

Consider first the case $f(x) = \sin kx$. From (3.19), the term $2e^{-\gamma|z|}$ in (3.39) makes a contribution $g_1(X)$ to $g(X)$ given by

$$\left(\gamma^2 + k^2\right) g_1(X) = 4\gamma \sin kX - 4\gamma e^{-\gamma L} \sinh \gamma X \left[\sin kL + \frac{k}{\gamma} \cos kL\right], \tag{3.40}$$

while the term $-e^{-2\gamma|z|}$ makes a contribution $g_2(X)$ given by

$$\left(4\gamma^2 + k^2\right) g_1(X) = -4\gamma \sin kX - 4\gamma e^{-2\gamma L} \sinh 2\gamma X \left[\sin kL + \frac{k}{2\gamma} \cos kL\right]. \tag{3.41}$$

Upon forming the sum $g(X) = g_1(X) + g_2(X)$, it becomes clear that the coefficient of $\sinh \gamma X$ vanishes if kL obeys $\gamma L \sin kL + kL \cos kL = 0$, and that the coefficient of $\sinh 2\gamma X$ vanishes if kL obeys $2\gamma L \sin kL + kL \cos kL = 0$. kL ($\neq 0$) cannot be chosen so that both coefficients vanish simultaneously. Hence $f(x) = \sin kx$ is not an eigenfunction.

A similar treatment may be applied in the case of $f(x) = \cos kx$. The two conditions $kL \sin kL - \gamma L \cos kL = 0$ and $kL \sin kL - 2\gamma L \cos kL = 0$ cannot be satisfied simultaneously, so $f(x) = \cos kx$ is not an eigenfunction.

The non-existence of either symmetric or antisymmetric sinusoidal eigenfunctions with the double exponential kernel (3.39) is consistent with the 7×7 results for the corresponding case (vi) of section 3(a). [Note that δ in case (vi) corresponds to $e^{-\gamma \Delta x}$, where Δx is the separation of gridpoints in the 7-point discretization.]

Another case that can be examined analytically is the second order regressive variation

$$K\left(|z|\right) = \left(1 + \frac{|z|}{\beta}\right) e^{-\alpha|z|}. \tag{3.42}$$

(See Daley (1991), p117, for a 2-dimensional variation of this type.) This kernel has the same gross features (non-negativity and smoothness) as the double exponential (3.39). No sinusoidal eigenfunctions, either symmetric or antisymmetric, occur.

From the cases investigated, it seems that sinusoidal eigenfunctions may be found if the kernel is salient (see Figure 2), but only in special circumstances if the kernel is smooth. (The occurrence of antisymmetric sinusoidal eigenfunctions for the parabolic kernel $K\left(|z|\right) = 1 - \beta^2 z^2$ illustrates one such special circumstance.) That the existence of a discontinuity of kernel slope is not a *sufficient* condition for the existence of sinusoidal eigenfunctions may be shown by repeating the linear kernel calculation with $2\alpha L > 1$ and $K\left(|z|\right) = \max\left\{1 - \alpha\,|z|\,,\ 0\right\}$ (so that K is positive semi-definite; this is a conventional "triangular" weighting). No sinusoidal eigenfunctions are found.

4 Semi-infinite domains

In place of (2.5), we have in the semi-infinite case

$$g(X) = \int_0^\infty K\left(|x - X|\right) f(x)\, dx = \int_{-X}^\infty K\left(|z|\right) f(z + X)\, dz. \tag{4.1}$$

For the exponential kernel $K\left(|z|\right) = e^{-\alpha|z|}$, (4.1) gives

$$g(X) = \left(\alpha^2 + k^2\right)^{-1} \left[2\alpha \sin kX + ke^{-\alpha X}\right] \tag{4.2}$$

if $f(x) = \sin kx$, and

$$g(X) = \left(\alpha^2 + k^2\right)^{-1} \left[2\alpha \cos kX - \alpha e^{-\alpha X}\right] \tag{4.3}$$

if $f(x) = \cos kx$. Sinusoids are therefore approximately eigenfunctions at large x ($x \gg \alpha^{-1}$), as one would expect, but not in the whole half plane $x > 0$. Similar results are obtained for the (salient) piece-wise linear kernel and with the (smooth) parabolic and double exponential kernels. Although we have examined only specific kernels, it is clear that the occurrence of eigenfunctions that are sinusoidal given some appropriate choice of kernel should not be assumed.

5 Mixed domains

Consider first a 2D Cartesian (x, y) "channel" domain which is cyclic in the direction of x and finite in the direction of y. The continuous integral eigenproblem is

$$\int\int K(x - X,\ y - Y) f(x, y) dx dy = \lambda f(X, Y). \tag{5.1}$$

If the kernel K is separable, i.e. if $K(x - X,\ y - Y) = K_1(x - X)K_2(y - Y)$, and we seek separable eigenfunctions $f(x, y) = f_1(x)f_2(y)$, then (5.1) may be written as

$$\int K_1(x - X) f_1(x) dx \int K_2(y - Y) f_2(y) dy = \lambda f_1(X) f_2(Y). \tag{5.2}$$

If f_1 and f_2 obey the 1D integral equations

$$\int K_1(x - X) f_1(x) dx = \lambda_1 f_1(X) \tag{5.3}$$

and

$$\int K_2(y - Y) f_2(y) dy = \lambda_2 f_2(Y), \tag{5.4}$$

then $f(x, y) = f_1(x)f_2(y)$ is an eigenfunction of (5.2) and hence of (5.1), with eigenvalue $\lambda = \lambda_1\lambda_2$. Eigenfunctions that are sinusoidal in both the x and y directions can thus be constructed by choosing a kernel K_2 that gives sinusoidal eigensolutions of (5.2) (in the knowledge that the variation in the x direction will be sinusoidal because that direction is cyclic). Alternatively, eigenfunctions that are sinusoidal only in the x direction can be

constructed by choosing a kernel K_2 that does not give sinusoidal solutions of (5.2). The argument is readily extended to 3D. Mixed-domain, separable-kernel eigen-problems can be solved as a product of problems in domains of lower dimension.

An important case in which this reasoning can be applied is the spherical annulus - in which the radial domain is finite (and spherical surfaces cyclic). Homogeneous covariance eigenfunctions in this 3D domain may be found as products of spherical harmonics (see Part I) and radial/vertical functions (which may or may not be sinusoidal, depending on the vertical structure of the separable homogeneous covariance function). Similar remarks apply to a domain which is bounded below but not above by a sphere; for this case, however, we have not identified kernels for which the radial/vertical variation of the eigenfunctions would be sinusoidal.

6 Discussion

In this paper we have continued an exploration of the conditions under which covariance matrices representing homogeneous, symmetric errors have sinusoidal eigenvectors. Whereas in Part I only cyclic domains were examined, here in Part II we have investigated non-cyclic domains - infinite, semi-infinite and finite. As in Part I we have exploited the status of covariance matrix eigen-problems as discretizations of certain integral equation eigen-problems. This gives a grid-independent guiding principle and mathematical basis.

In infinite domains, sinusoidal eigenfunctions are ubiquitous, the corresponding eigenvalues being simply the Fourier cosine transforms of the covariance function. In semi-infinite domains we have not found strictly sinusoidal eigenfunctions. In finite domains, sinusoidal eigenfunctions occur for certain families of covariance functions, but not for others. Our investigation has been experimental rather than systematic, so firm conclusions cannot be drawn, but the *suggestion* of our results is that the occurrence of sinusoidal eigenfunctions for a finite domain is closely associated with "salient" symmetric covariance functions - those having a central discontinuity of slope. The existence of such a discontinuity is, however, neither a necessary nor a sufficient condition for the occurrence of sinusoidal eigenfunctions. Investigation of these issues, making use of techniques for analysing integral equations (as described by Porter and Stirling (1990) and by Srivastava and Buschman (1992)) is a promising area for future study.

Other possibilities also warrant further study. Some cases in which eigenfunctions are not sinusoidal may yet be handled analytically. Perturbation problems in which the sinusoidal cases are taken as the zero-order state can also be envisaged. The known correspondence between integral equations and differential equations should also be explored; it is hinted at in many of the results presented in this paper - perhaps most strongly by the simple tridiagonal form, suggestive of a discretized second derivative, of the matrix T_{lin}^{-1} (see Appendix).

One way of ensuring sinusoidal eigenfunctions in a finite domain is to force the problem to be cyclic on that scale. This involves making the kernel cyclic, which in discrete cases means replacing the Toeplitz covariance matrices by related circulant forms. The approach is described and studied by Healy and White (2004), who find that the approximations introduced are acceptable for many purposes in 1D retrievals.

We have shown that mixed cyclic/non-cyclic domains support sinusoidal eigenfunctions

when kernels are separable into appropriate symmetric functions. Regarding such kernels, it should be noted (see section 3 of Part I) that the corresponding homogeneous covariance is separably symmetric but not radially symmetric (and hence not isotropic).

As a corpus, the results presented in this paper and in Part I offer a simple but broad analytical framework for understanding, interpreting and constructing data assimilation schemes. These schemes may be of considerable complexity. It is helpful to be able to work through their procedures analytically on the assumption of homogeneous and symmetric error covariance. Many schemes try to rise above such assumptions, but it is revealing to note the extent to which they assume behaviour which is strictly applicable only when error covariance is homogeneous and symmetric. Viewed from this angle, our analysis emphasises conditions under which such an assumption is not strictly valid.

At a qualitative level, our results provide useful background as to why data assimilation schemes treat horizontal and vertical variations of error covariance in different ways (see Lorenc *et al.* (2000), pp2999-3000 and Ingleby (2001), p218). For homogeneous, symmetric error covariance, the eigenfunctions are surface spherical harmonics in the horizontal (see Part I), but are sinusoidal in the vertical only for certain (usually "salient") covariance profiles. Hence a different treatment of horizontal and vertical variations is to be expected.

Our results are also useful in specific respects relating to data assimilation. In Part I (section 2), nine aspects of the cyclic domain case were listed. Of these, we shall for brevity mention the analogue of only one here: the role of the eigenvalues of the covariance matrix in determining the conditioning of the untransformed variational analysis problem. If the range of the eigenvalues is small, then this problem is well posed, but if their range is large then the problem is ill posed. In the finite domain case, with an exponential kernel, the eigenvalues are precisely equal to the standard Fourier cosine transform of the kernel. In this case, at least, the range of eigenvalues is the same as if the domain had been infinite.

The sinusoidal eigenvector cases to which we have drawn attention are useful because of their analytical tractability. An eigen-problem of this type - corresponding to the "exponential" case examined here in section 3 and in the Appendix - was analysed by Rodgers (2000) (pp52, 218), but perhaps it has not been widely appreciated that non-diagonal error covariance matrices exist which can be treated analytically. Such cases not only aid understanding; they enable the assessment of error characteristics to be improved by supplying a tractable *co*variance model (rather than the restricted variance model supplied by diagonal matrices). An example of this application is described by Healy and White (2004).

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Appendix: $N \times N$ symmetric Toeplitz matrices having sinusoidal eigenvectors

Consider the $N \times N$ symmetric, tridiagonal Toeplitz matrix

$$\mathbf{T}_{tri} = \begin{pmatrix} 1 & a & . & ... & . \\ a & 1 & a & ... & . \\ . & a & 1 & ... & . \\ \vdots & \vdots & \vdots & & \vdots \\ . & . & ... & a & 1 \end{pmatrix} \tag{6.1}$$

in which each element along the leading diagonal is 1, each entry along the adjacent diagonals is a, and every other entry is 0. Suppose that N is odd, i.e. $N = 2M + 1$ for some integer $M > 0$, and label the components x_m of a putative eigenvector $\mathbf{x}$ from $-M$ to $= M$:

$$\mathbf{x} = \left(x_{-M},\, x_{-(M-1)},\, ...,\, x_{-1},\, x_0,\, x_1, ..., x_{M-1},\, x_M\right)^T. \tag{6.2}$$

[The case of even N can be treated in a similar way.] Except for $m = \pm M$, the mth component of $\mathbf{T}_{tri}\mathbf{x}$ is

$$\left(\mathbf{T}_{tri}\mathbf{x}\right)_m = ax_{m-1} + x_m + ax_{m+1}. \tag{6.3}$$

Consider the family of symmetric sinusoids having $x_m = \cos m\alpha$ $(-M \leq m \leq M)$ where α is a real parameter. For this family (6.3) gives

$$\left(\mathbf{T}_{tri}\mathbf{x}\right)_m = \left[1 + 2a\cos\alpha\right]\cos m\alpha = \left[1 + 2a\cos\alpha\right]x_m \quad (-M < m < M) \tag{6.4}$$

Thus $x_m = \cos m\alpha$ is an eigenvector of $\mathbf{T}_{tri}$, with eigenvalue $1 + 2a\cos\alpha$, so long as (6.4) is obeyed for $m = \pm M$ as well as for $-M < m < M$. But

$$\left(\mathbf{T}_{tri}\mathbf{x}\right)_{\pm M} = x_{\pm M} + ax_{\pm(M-1)} = \cos M\alpha + a\cos\left(M-1\right)\alpha \tag{6.5}$$

i.e.

$$\left(\mathbf{T}_{tri}\mathbf{x}\right)_{\pm M} = \left[1 + 2a\cos\alpha\right]\cos M\alpha - a\cos\left(M+1\right)\alpha. \tag{6.6}$$

Hence if $x_m = \cos m\alpha$ is an eigenvector of $\mathbf{T}_{tri}$, α must obey $\cos\left(M+1\right)\alpha = 0$. This condition determines $M + 1$ allowable values of α:

$$\alpha = \alpha_n = \frac{(2n+1)}{2(M+1)}\pi, \quad n = 0, 1, 2, ...M. \tag{6.7}$$

The corresponding eigenvalues of $\mathbf{T}_{tri}$ are $1 + 2a\cos\alpha_n$.

A similar analysis may be applied to the family of antisymmetric sinusoids having $x_m = \sin m\beta$ $(-M \leq m \leq M)$ where β is a real parameter. $x_m = \sin m\beta$ is an eigenvector of $\mathbf{T}_{tri}$ with eigenvalues $1 + 2a\cos\beta$ so long as:

$$\beta = \beta_n = \frac{n}{(M+1)}\pi, \quad n = 1, 2, ...M. \tag{6.8}$$

According to (6.7) and (6.8), there are $2M+1$ independent eigenvectors; because $\mathbf{T}_{tri}$ is symmetric they are orthogonal and complete. Even the gravest symmetric eigenvector (corresponding to $n=0$ in (6.7)) is not simply a constant (i.e. it varies with m).

The following variant of $\mathbf{T}_{tri}$ can be analysed in a similar way:

$$\mathbf{T}_{trivar} = \begin{pmatrix} q & a & . & ... & p \\ a & 1 & a & ... & . \\ . & a & 1 & ... & . \\ \vdots & \vdots & \vdots & & \vdots \\ p & . & ... & a & q \end{pmatrix}. \tag{6.9}$$

Elements p which may be non-zero occur at the extremes of the secondary diagonal in (6.9), and the elements q at the extremes of the leading diagonal are not necessarily equal to unity. Orthogonal, sinusoidal eigenvectors of $\mathbf{T}_{trivar}$ exist of the form $x_m = \cos m\alpha$ and $x_m = \sin m\beta$. In the symmetric case the eigenvalues are, as before, $1+2a\cos\alpha$, but values of α are determined as solutions of the transcendental equation

$$(1-p-q)\cos\alpha M + a\cos\alpha\,(M+1) = 0. \tag{6.10}$$

In the anti-symmetric case, the eigenvalues are $1+2a\cos\beta$, where

$$(1+p-q)\sin\beta M + a\sin\beta\,(M+1) = 0. \tag{6.11}$$

Consider now the "exponential" symmetric Toeplitz matrix

$$\mathbf{T}_{exp} = \begin{pmatrix} 1 & a & a^2 & ... & a^{N-1} \\ a & 1 & a & ... & a^{N-2} \\ a^2 & a & 1 & ... & a^{N-3} \\ \vdots & \vdots & \vdots & & \vdots \\ a^{N-1} & a^{N-2} & ... & a & 1 \end{pmatrix}. \tag{6.12}$$

As observed by Rodgers (2000) [see p218], the inverse of $\mathbf{T}_{exp}$ is tridiagonal. It is

$$\mathbf{T}_{exp}^{-1} = \frac{1}{(1-a^2)} \begin{pmatrix} 1 & -a & . & ... & . \\ -a & 1+a^2 & -a & ... & . \\ . & -a & 1+a^2 & ... & . \\ \vdots & \vdots & \vdots & & \vdots \\ . & . & ... & -a & 1 \end{pmatrix}, \tag{6.13}$$

which is a constant multiple of a matrix of the form (6.9) (with $p=0$). Hence $\mathbf{T}_{exp}^{-1}$ has sinusoidal eigenvectors. But a matrix and its inverse have the same eigenvectors. So $\mathbf{T}_{exp}$ has sinusoidal eigenvectors - the "truncated sinusoids" noted by Rodgers (2000), pp52.

One way of motivating (6.13) is to derive the inverse for a specific case (say 5×5) by row manipulation. In this method (see Mirsky 1955), a sequence of elementary row operations $\mathbf{E}_r$ is sought which reduces the matrix to be inverted to the unit matrix $\mathbf{I}$:

$$\mathbf{I} = \mathbf{E}_n....\mathbf{E}_r.....\mathbf{E}_2\mathbf{E}_1\mathbf{T}_{exp} = \mathbf{E}_n....\mathbf{E}_r.....\mathbf{E}_2\mathbf{E}_1\mathbf{I}\mathbf{T}_{exp}. \tag{6.14}$$

(An elementary row operation replaces any row of the current matrix by any non-trivial linear combination of the rows.) Applying the sequence of operations $\mathbf{E}_n....\mathbf{E}_r.....\mathbf{E}_2\mathbf{E}_1$ to the unit matrix thus gives $\mathbf{T}_{exp}^{-1}$.

The method can be applied to invert the following $(2N+1)\times(2N+1)$ "linear" symmetric Toeplitz matrix:

$$\mathbf{T}_{lin} = \begin{pmatrix} 1 & 1-\delta & 1-2\delta & ... & 1-2N\delta \\ 1-\delta & 1 & 1-\delta & ... & 1-(2N-1)\delta \\ 1-2\delta & 1-\delta & 1 & ... & 1-(2N-2)\delta \\ \vdots & \vdots & \vdots & & \vdots \\ 1-2N\delta & 1-(2N-1)\delta & ... & 1-\delta & 1 \end{pmatrix}. \tag{6.15}$$

The inverse is also of symmetric Toeplitz form:

$$\mathbf{T}_{lin}^{-1} = \frac{1}{2\delta}\begin{pmatrix} 1+\gamma_N & -1 & . & ... & \gamma_N \\ -1 & 2 & -1 & ... & . \\ . & -1 & 2 & ... & . \\ \vdots & \vdots & \vdots & & \vdots \\ \gamma_N & . & ... & -1 & 1+\gamma_N \end{pmatrix} \tag{6.16}$$

where

$$\gamma_N \equiv \frac{\delta}{2(1-N\delta)}. \tag{6.17}$$

The inverse (6.16) is equal to a constant multiple of a matrix of the form (6.9). So both $\mathbf{T}_{lin}^{-1}$ and $\mathbf{T}_{lin}$ have sinusoidal eigenvectors.

The $N \times N$ "uniform" matrix

$$\mathbf{T}_{uni} = \begin{pmatrix} 1 & a & a & ... & a \\ a & 1 & a & ... & a \\ a & a & 1 & ... & a \\ \vdots & \vdots & \vdots & & \vdots \\ a & a & ... & a & 1 \end{pmatrix} \tag{6.18}$$

can be treated by direct algebraic solution of the eigenvalue problem

$$\det\left(\mathbf{T}_{uni} - \lambda\mathbf{I}\right) = 0. \tag{6.19}$$

By manipulation of $\det\left(\mathbf{T}_{uni} - \lambda\mathbf{I}\right)$ into upper triangular form, (6.19) can be rewritten as

$$\left(1+(N-1)a-\lambda\right)\left(1-a-\lambda\right)^{N-1} = 0. \tag{6.20}$$

Hence $\mathbf{T}_{uni}$ has a non-degenerate eigenvalue $\lambda = 1+(N-1)a$, and $(N-1)$ degenerate eigenvalues $\lambda = 1-a$. The eigenvector associated with the the non-degenerate eigenvalue has every element equal (to $N^{-1/2}$ when normalised), and can be recognised simply by inspection of (6.18) and (6.19). The eigenvectors associated with the degenerate eigenvalues can be any vector whose elements sum to zero; it is convenient to apply the Schmidt orthogonalization procedure to obtain them as sines and cosines. The sinusoidal character of the eigenvectors of $\mathbf{T}_{uni}$ also follows from the fact that it is a circulant matrix as well as a Toeplitz matrix.

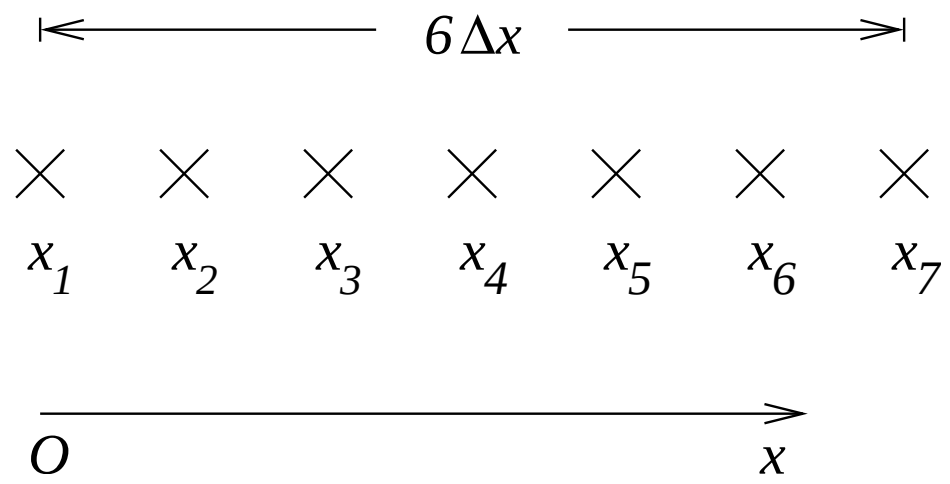

Figure 1: Points x_1, x_2, x_3, x_4, x_5, x_6, x_7 equally-spaced in a 1D domain of length $6\Delta x$

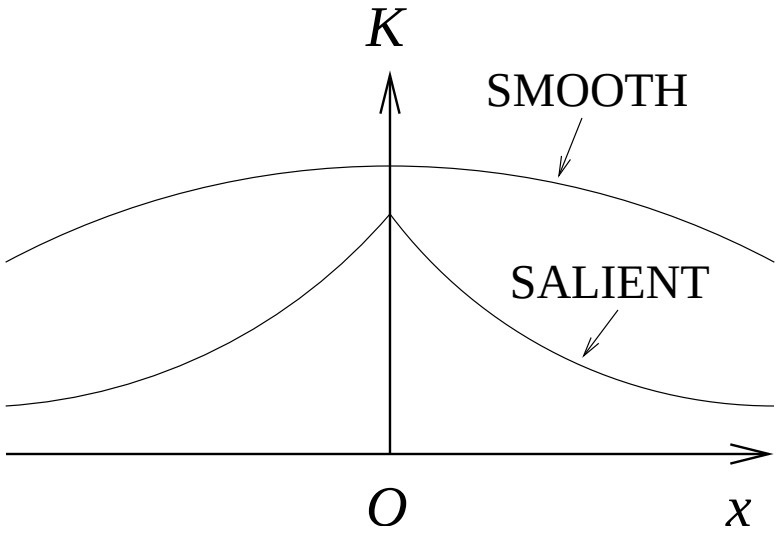

Figure 2: Illustrating smooth and salient symmetric kernel functions $K(x) = K(|x|)$